Imidazole, 1-(p-nitrophenyl)-

Other names:	1-(4-Nitrophenyl)-1H-imidazole 1H-Imidazole, 1-(4-nitrophenyl)- 1-(4-Nitrophenyl)imidazole
Inchi:	InChI=1S/C9H7N3O2/c13-12(14)9-3-1-8(2-4-9)11-6-5-10-7-11/h1-7H
InchiKey:	PUCOOPJLAXJKOO-UHFFFAOYSA-N
Formula:	C9H7N3O2
SMILES:	O=[N+]([O-])c1ccc(-n2ccnc2)cc1
Mol. weight [g/mol]:	189.17
CAS:	2301-25-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.780		Crippen Method
mcvol	131.830	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2301259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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